Structure Determination of the Si(111)(√3x√3)R30°-B Structure Using Photoelectron Diffraction

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The influence of dopants on the properties of a semiconductor are of interest both from the scientific and technological points of view. Due to the presence of the solid-vacuum interface one might expect the properties of the near-surface region to be different from those of the underlying bulk semiconductor material. Annealing of a heavily boron-doped Si(111) crystal, for example, gives rise to a (√3x√3)R30° phase in which the concentration of boron is much higher than in the bulk material. Moreover, a surface alloy is formed even though boron and silicon are immiscible in the bulk. The existence of this (√3x√3)R30° phase is well known, but only recently has the rather unusual atomic geometry been quantitatively determined by LEED and surface x-ray diffraction [1,2]. It was found that the boron adopts the substitutional site directly underneath a silicon adatom. All surface (√3x√3)R30° adatoms are therefore Si, in contrast to similar structures formed by other group III elements.

Since both LEED and x-ray diffraction are rather insensitive to the exact local atomic arrangement around the weakly-scattering boron atom, we have conducted a scanned-energy mode photoelectron diffraction (PhD) study of the (√3x√3)R30° structure using the B 1s photoemission signal. The local nature of this probe enables the boron atom position to be determined very accurately. B 1s photoelectron diffraction modulation spectra were obtained using the same methodology we have previously established in many similar studies at the BESSY facility in

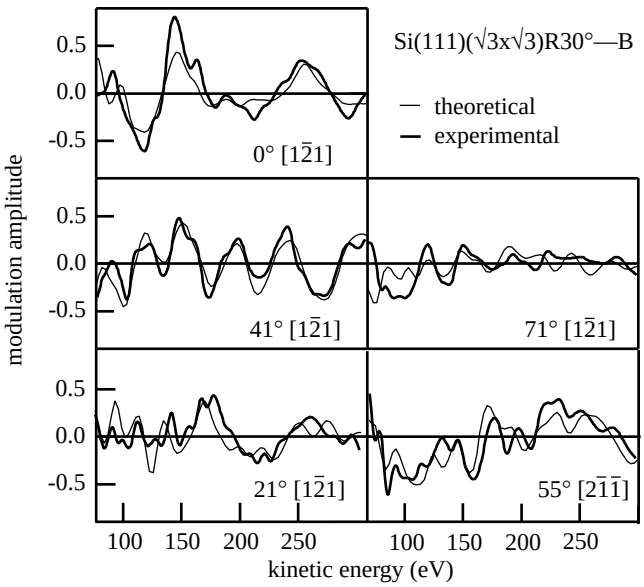

Figure 1. Experimental PhD modulation spectra for the Si(111) (√3x√3)R30°-boron phase (bold lines) together with the simulated spectra for the optimum structure shown in Fig. 2.

Berlin [3]. Spectra were measured at five different emission directions over the kinetic energy range 60-310 eV on beamline 7.0.1. The high photon flux and spectral resolution enabled us to exploit the full energy range, despite the overlap of the B 1s photoemission peak with an intense substrate Auger electron emission peak at a kinetic energy of around 90 eV. A good photon energy resolution is essential to separate the B 1s signal from the Auger background in this energy region.

Fig. 1 shows the experimental PhD modulation spectra measured in five different emission directions. The structure determination was performed by comparing the experimental data (bold curves) with simulated data (faint curves) using a multiple scattering formalism. The model geometry is optimised using an automated search algorithm for the best fit between experiment and theory.

A schematic drawing of the parameters varied and their optimum values is shown in Fig.2. The structural parameters agree with the previous LEED and x-ray diffraction measurements within the precision of the techniques. However, the key parameters, such as the bondlengths to the nearest neighbour atoms of the boron in the different layers, could be determined with much higher precision than hitherto. Full details of the optimum structure will be submitted for publication shortly.

ACKNOWLEDGEMENTS
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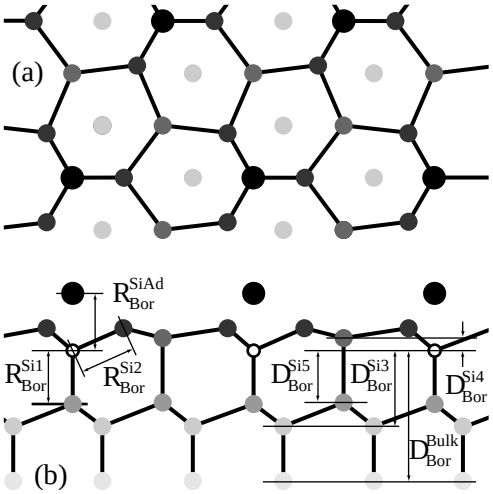

R_{Bor}^{Si1} =(2,3±0.1)Å
R_{Bor}^{Si2} =(2,3±0,5)Å
R_{Bor}^{SiAd} =(2,2±0,2)Å
D_{Bor}^{Si3} =(2,7±0,1)Å
D_{Bor}^{Si4} =(0,4±0,2)Å
D_{Bor}^{Si5} =(1,9±0,1)Å
D_{Bor}^{Bulk} =(5,2±0,2)Å

Figure 2. Structural parameters for the Si(111)-(√3x√3)R30° boron phase and their optimised values.